# Adams representation and localization in a magnetic field

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The localization problem of a Bloch electron in a magnetic field is investigated by using the concepts of the Adams representation and of von Neumann lattices. Bloch functions in a magnetic field are derived, and their properties are established. The magnetic Adams representation, based on these functions, is constructed. It is characterized by a magnetic band index and a magnetic quasimomentum  $\vec{\kappa}$ , and is analogous to the Adams representation in the Bloch theory. It is shown that the problem of localization in a magnetic field is closely related to the corresponding problem in the theory of von Neumann lattices.

#### I. INTRODUCTION

The Bloch theory<sup>1</sup> is based on the invariance of a crystalline lattice under translations. Because of this invariance a conserved quasimomentum (or crystal momentum)  $\vec{k}$  exists in ideal solids. In the presence of a uniform magnetic field  $\vec{H}$  the solid is invariant under magnetic translations.<sup>2,3</sup> The latter invariance leads to a conserved quantity  $\vec{\kappa}$ , which is connected with the center of magnetic orbits. As a consequence of translational invariance the energy spectrum displays a band structure both for  $\dot{H}=0$  and  $\vec{H} \neq 0$ . The existence of bands in the Bloch theory (H=0) was used by Adams in order to develop what is called the Adams, or the crystal-momentum, representation<sup>4</sup> (CMR). This representation has provided a suitable framework for studying a variety of phenomena in condensed matter. $^{5-7}$  Qualitatively, the usefulness of the CMR follows from the fact that, because of the energy gaps in the spectrum, most of the physics takes place in one band or in a small number of bands. A similar situation should also prevail when a magnetic field is present, and then one speaks of magnetic bands, or broadened Landau levels.<sup>8-10</sup> It should therefore be of interest to develop the Adams representation for Bloch electrons in a magnetic field.

The translation group and the magnetic translation group have a number of features in common. They both are built on the discrete lattices of solids, lead to conserved quantities (k for the translations and  $\vec{\kappa}$  for the magnetic translations), and, finally, the energy spectrum in both cases has a band structure. However, on a deeper level there turns out to be a substantial difference between these two symmetries. It is by now well known that the magnetic translation group is very different in its basic structure from the usual translation group.<sup>11-13</sup> In addition, from the point of view of the dynamics the magnetic field introduces drastic changes since it leads to a singular perturbation in the Hamiltonian.<sup>14</sup>

A general form for the eigenfunctions of a Bloch electron in a magnetic field can be written on the basis of group-theoretical considerations.<sup>2,3,15</sup> These eigenfunctions are labeled by the magnetic  $\vec{k}$  vector  $(\vec{\kappa}$  vector in this paper), which specifies an irreducible representation of the magnetic translation group, and by an index indicating the magnetic band, or broadened Landau level.<sup>8</sup> The group-theoretical approach can be well analyzed on the basis of the kqrepresentation.<sup>16,17</sup> Recently,<sup>18</sup> this representation was used for writing down expressions for the Bloch functions in a magnetic field and for numerical calculations of the energy spectrum.

An alternative approach to the problem of an electron in a magnetic field can be achieved by means of canonical transformations.<sup>19</sup> In the latter approach the Hamiltonian assumes an explicit harmonic-oscillator form. In particular, the infinite degeneracy of a Landau level is displayed quite well in the transformed coordinates. Canonical transformation methods have also been used<sup>20</sup> to find an interesting similarity between Pippard networks of Dingle functions<sup>9</sup> and von Neumann lattices of coherent states.<sup>21</sup> This similarity follows from the fact that both the Pippard network and the von Neumann lattice are generated from a discrete set of translations in phase space. In the case of the Pippard network this set consists of the magnetic translations, while for the von Neumann lattice it consists of translations in the x-p (coordinatemomentum) phase space. Since the kq representation<sup>16</sup> is based on exactly this latter type of translation, it should give a connection between Pippard networks and von Neumann lattices.

The classical Pippard network<sup>9</sup> is based on a set of Dingle functions, which are well-localized in

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space. The problem of completeness of this set relative to a Landau level is closely related to the corresponding problem for sets on a von Neumann lattice.<sup>20</sup> In the presence of a periodic potential the Dingle functions will be replaced by some more general set of localized orbitals.<sup>22–27</sup> These latter orbitals are related to the localized functions for a Bloch electron in a magnetic field. When  $\vec{H}=0$ , these are the Wannier functions or, more generally, the localized functions for the Bloch problem.<sup>28</sup> While the problem of Wannier functions ( $\vec{H}=0$ ) has been investigated in a number of papers,<sup>29,30</sup> there is no comparable work on the problem of localized orbitals in a magnetic field.

In this paper properties of sets on von Neumann lattices are used for investigating the problem of localization of a Bloch electron in a magnetic field. We restrict ourselves to the case of rational magnetic fields. In Sec. II, Bloch functions in a magnetic field are derived, and their properties are considered. In Sec. III we construct the magnetic Adams representation, based on these functions. When restricted to a single magnetic band, the Adams representation essentially reduces to a kq representation in the two components of  $\vec{\kappa}$  perpendicular to  $\vec{H}$ . In Sec. IV the problem of localization of magnetic orbitals is investigated by using the concepts of the Adams representation and of von Neumann lattices. A Pippard network is introduced, reproducing a single magnetic band. Magnetic Wannier functions on this network are obtained, and the concept of localization of magnetic orbitals is then discussed. It is shown that localization is accompanied by nonorthogonality.

# **II. BLOCH FUNCTIONS IN A MAGNETIC FIELD**

The Hamiltonian of an electron (of charge -e and mass M) moving under the influence of a periodic potential  $V(\vec{r})$  and a uniform magnetic field  $\vec{H}$  is

$$H = \frac{\vec{\Pi}^2}{2M} + V(\vec{r}) , \qquad (1)$$

where  $\vec{\Pi}$  is the kinetic momentum

$$\vec{\Pi} = \vec{p} + \frac{1}{2}\vec{\beta} \times \vec{r} , \quad \vec{\beta} = \frac{e}{c}\vec{H}$$
(2)

written in the symmetric gauge (which is adopted in this paper). Let the basis vectors of the lattice be  $\vec{a}_1$ ,  $\vec{a}_2$ , and  $\vec{a}_3$ . It is assumed in what follows that  $\vec{H}$  is parallel to  $\vec{a}_3$ , and that it satisfies the rationality condition<sup>9,11</sup>

$$\frac{e\vec{H}}{hc} \cdot \vec{a}_1 \times \vec{a}_2 = \frac{1}{N} , N \text{ positive integer }.$$
(3)

What condition (3) means is that it is possible to

have a superlattice with basis vectors  $\vec{b}_1 = N_1 \vec{a}_1$  and  $\vec{b}_2 = N_2 \vec{a}_2$  ( $N_1$  and  $N_2$  are integers satisfying  $N_1 N_2 = N$ ), such that the magnetic flux through the unit cell built on  $\vec{b}_1$  and  $\vec{b}_2$  is exactly the quantum of flux, hc / e. It is easily verified, using (3), that the two operators (magnetic translations)

$$T(\vec{\mathbf{b}}_{j}) = \exp\left[\frac{i}{\hbar} \vec{\Pi}_{c} \cdot \vec{\mathbf{b}}_{j}\right], \quad j = 1,2$$
(4)

where

$$\vec{\Pi}_{c} = \vec{p} - \frac{1}{2}\vec{\beta} \times \vec{r} , \qquad (5)$$

commute, and that they also commute with the Hamiltonian H in (1).

We want to study the nature of the simultaneous eigenfunctions of (1) and (4). For the sake of clarity, let us restrict ourselves to the case of a twodimensional rectangular lattice perpendicular to  $\vec{H}$ , and neglect the motion along  $\vec{H}$ . Our results can be extended to more general cases without much difficulty. Thus, let the lattice vectors  $\vec{a}_1$  and  $\vec{a}_2$  be directed along the x and y axes, respectively, of a coordinate system (x,y). We will now describe the problem in terms of new coordinates defined by the canonical transformation<sup>20</sup>

$$Q = p_{x} / \beta + y / 2 , \quad P = p_{y} - \beta x / 2 ,$$
  

$$\bar{Q} = p_{y} / \beta + x / 2 , \quad \bar{P} = p_{x} - \beta y / 2 ,$$
(6)

which preserves the commutation relations between the position and momentum coordinates

$$[Q,P] = [\overline{Q},\overline{P}] = i\hbar, \qquad (7)$$

and all the other pairs of operators from (6) commute. The advantage of using the coordinates (6) is that they are simply related to the components of the operators  $\vec{\Pi}$  and  $\vec{\Pi}_c$ , given by (2) and (5). In fact, one has

$$Q = y_0 = \Pi_{cx} / \beta , \quad P = -\beta x_0 = \Pi_{cy} ,$$
  
$$\overline{Q} = \Pi_y / \beta , \quad \overline{P} = \Pi_x ,$$

where  $(x_0, y_0)$  corresponds to the center of the magnetic orbit.<sup>31</sup> In what follows we shall work in the  $\overline{PP}$  representation, details of which are given in the Appendix.

Let us write the Hamiltonian  $H_0$  (for V=0) and the magnetic translations (4) in the new coordinates<sup>20</sup>:

$$H_0 = \frac{\vec{\Pi}^2}{2M} = \frac{1}{2M} (\beta^2 \bar{Q}^2 + \bar{P}^2) , \qquad (8)$$

$$T(\vec{b}_1) = \exp\left[\frac{i}{\hbar}\beta Q b_1\right], \quad T(\vec{b}_2) = \exp\left[\frac{i}{\hbar}P b_2\right].$$
(9)

Because of the absence of the Q,P canonical pair in (8), a general eigenfunction of  $H_0$  assumes the following form in the  $\overline{P}P$ -representation [a superscript (0) will indicate the case V=0]

$$\psi^{(0)}(\bar{P}, P) = f_l(\bar{P})g(P) , \qquad (10)$$

where  $f_l(\bar{P})$  is an oscillator function in  $\bar{P}$ , corresponding to the energy

$$\epsilon_l = (l + \frac{1}{2})\hbar\omega_c$$
,  $\omega_c = \frac{eH}{Mc}$ ,  $l = 0, 1, \dots$  (11)

and g(P) is an arbitrary function of P. This arbitrariness in (10) is directly related to the well-known infinite degeneracy of the Landau levels [Eq. (11)].<sup>20</sup> One may consider several complete sets of functions g(P) spanning a given Landau level.<sup>31</sup> Thus, the set of Dingle functions<sup>20</sup>

$$\psi_{lp}^{(0)}(\bar{P},P) = f_l(\bar{P})f_p(P) , \ p = 0, 1, \dots$$
 (12)

 $[f_p(P)$  is an oscillator function in P] specifies the square of the radius vector for the orbit center:  $r_0^2 = (p + \frac{1}{2})\hbar/\beta$ .

We now choose g(P) as an eigenfunction of the magnetic translations (9). By doing so, (10) will become a simultaneous eigenfunction of (8) and (9). Because of (7) the magnetic translations (9) are essentially translations in the phase space defined by the Q-P plane.  $T(\vec{b}_1)$  gives a translation by  $-\beta b_1$ 

in P, while  $T(\vec{b}_2)$  gives a translation by  $b_2$  in Q. These translations in P and Q satisfy, because of (3), the relation

$$\beta b_1 b_2 = h . \tag{13}$$

By using the operators in (9) together with Eq. (13) one can define the kq representation<sup>16</sup> for the pair of canonical coordinates Q and P. The latter play the role of x and p (up to a constant) in the original kq representation. The eigenfunctions of the operators (9) assume, then, the following form:

$$\langle P \mid \vec{\kappa} \rangle = \sqrt{\hbar b_1 / 2\pi} \sum_{m = -\infty}^{\infty} e^{-i\kappa_1 m b_1} \times \delta(P - \hbar \kappa_2 - \beta m b_1)$$
(14)

where  $\vec{\kappa} \equiv (\kappa_1, \kappa_2)$  specifies the eigenvalues of the magnetic translations, corresponding to the eigenfunction (14), via the expressions

$$\exp(i\kappa_1b_1)$$
,  $\exp(i\kappa_2b_2)$ 

for  $T(\vec{b}_1)$  and  $T(\vec{b}_2)$ , respectively. With the normalization constant in (14), the following orthogonality relation is satisfied:

$$\int dP \langle \vec{\kappa} | P \rangle \langle P | \vec{\kappa'} \rangle = \hat{\Delta}(\vec{\kappa} - \vec{\kappa'}) \equiv \sum_{m} \delta(\kappa_1 - \kappa'_1 - (2\pi/b_1)m) \sum_{n} e^{-i\kappa_1 n b_1} \delta(\kappa_2 - \kappa'_2 - n(\beta/\hbar)b_1) .$$
(15)

By choosing (14) as g(P) we obtain the simultaneous eigenfunctions of (8) and (9):

$$\psi_{l\vec{\kappa}}^{(0)}(\vec{P},P) = f_{l}(\vec{P}) \langle P \mid \vec{\kappa} \rangle .$$
(16)

In this expression the x coordinate of the orbit center is determined up to a multiple of  $b_1$ , while the y coordinate is fixed up to a multiple of  $b_2$ . Thus the vector  $\vec{\kappa}$  gives the coordinates of the orbit center relative to the magnetic cell built on  $\vec{b}_1$  and  $\vec{b}_2$ . All the orbit centers in a magnetic cell are obtained by varying  $\vec{\kappa}$  in the magnetic Brillouin zone:

$$0 \le \kappa_1 < 2\pi/b_1 , 0 < \kappa_2 < (\beta/\hbar)b_1 \ (=2\pi/b_2) .$$
(17)

Next, we consider the case when a twodimensional periodic potential  $V(\vec{r})$  is present in the plane perpendicular to  $\vec{H}$ . Let us expand it in a

Fourier series,

$$V(\vec{\mathbf{r}}) = \sum_{m,n} v_{m,n} \exp(i\vec{\mathbf{K}}_{m,n} \cdot \vec{\mathbf{r}}) , \qquad (18)$$

where  $\vec{r} \equiv (x,y)$  is the radius vector and  $\vec{K}_{m,n}$  are vectors of the reciprocal lattice. The magnetic translations (9) commute with (1), and the simultaneous eigenfunctions  $\psi_{l\vec{k}}$  of H and of (9) must therefore contain the distribution (14). The most general form of  $\psi_{l\vec{k}}$  is

$$\psi_{l\vec{\kappa}}(\bar{P},P) = \varphi_{l\vec{\kappa}}(\bar{P}) \langle P \mid \vec{\kappa} \rangle , \qquad (19)$$

where  $\varphi_{l\vec{\kappa}}$  is to be determined from the Schrödinger equation with the Hamiltonian (1). Let us substitute (19) into the Schrödinger equation. By using the explicit expression for  $\vec{K}_{m,n}$  in Eq. (18), it is easily verified that  $\varphi_{l\vec{\kappa}}(\bar{P})$  satisfies the following eigenvalue problem:

$$\left[H_{0}+\sum_{m,n}v_{m,n}\exp\left[(iN/\hbar)(\hbar\kappa_{1}-\bar{P})na_{1}\right]\exp\left[(iN/\hbar)(\beta\bar{Q}-\hbar\kappa_{2})ma_{2}\right]\right]\varphi_{l\vec{\kappa}}(\bar{P})=\epsilon_{l}(\vec{\kappa})\varphi_{l\vec{\kappa}}(\bar{P}).$$
(20)

Apart from notation, Eq. (20) is identical with the one-dimensional equation that was derived before by a different method.<sup>32</sup> Recently, this equation was derived again on the basis of the kq representation.<sup>18</sup> Equation (20) is  $\vec{\kappa}$  dependent, and should give, for a fixed l, a continuous energy spectrum  $\epsilon_l(\vec{\kappa})$ , or a magnetic band. A band structure in the spectrum is a well-known feature of the Bloch problem (H=0). In the latter case, for each fixed quasimomentum one obtains a discrete spectrum of energies.<sup>33</sup> One should expect a similar situation to exist for  $H \neq 0$ , and for each  $\vec{\kappa}$  in Eq. (20) one should get a discrete set of energies. There is no exact proof of this statement. However, it is plausible because if the periodic potential is considered as a perturbation in Eq. (20), one obtains for each  $\vec{\kappa}$  a discrete spectrum.<sup>32,34</sup> Numerical calculations also show that the spectrum  $\epsilon_l(\vec{\kappa})$  for a fixed  $\vec{\kappa}$  is discrete.<sup>18</sup> Similarly, one should expect the solutions of Eq. (20) to be squareintegrable functions in the variable  $\overline{P}$ . This feature of the functions comes together with the abovementioned discreteness of the spectrum. An example of a square-integrable function is the oscillator function  $f_l(\overline{P})$  appearing in (16).

In Eq. (20)  $\vec{\kappa}$  varies over the magnetic Brillouin zone (17). However, as is seen from Eq. (20), its solutions are periodic in  $\kappa_1$  and  $\kappa_2$  with the periods  $2\pi/Na_1$  and  $2\pi/Na_2$ , respectively. These periods define a unit cell which is N times smaller than that given by (17). This fact leads to the well-known Nfold degeneracy in a magnetic band<sup>2,3</sup> and to the following periodicity conditions obeyed by the eigenfunctions (19) [or (16)]:

$$\psi_{l,\kappa_1+2\pi/b_1,\kappa_2}(\bar{P},P) = \psi_{l,\vec{\kappa}}(\bar{P},P) , \qquad (21a)$$

$$\psi_{l,\kappa_1,\kappa_2+\beta b_1/\hbar}(\overline{P},P) = e^{i\kappa_1 b_1} \psi_{l,\vec{\kappa}}(\overline{P},P) . \qquad (21b)$$

Conditions (21) are quite different from those satisfied by usual Bloch functions  $\psi_{m\,\vec{k}}$  (*m* is the band index) with respect to the quasimomentum  $\vec{k}$ . Indeed, Bloch functions can be made periodic in  $\vec{k}$ in the reciprocal lattice,<sup>35</sup> while the eigenfunctions (19) must satisfy the Bloch-periodicity condition (21b) in  $\kappa_2$ . One may shift this Bloch periodicity from  $\kappa_2$  to  $\kappa_1$  by multiplying (19) by a proper (continuous in  $\vec{\kappa}$ ) phase factor, but one cannot eliminate it completely. This characteristic of the eigenfunctions (19) is a consequence of the fact that they are eigenfunctions of translations in phase space and not in ordinary space as in the case of Bloch functions. Despite the fact that the magnetic translations (4) commute in the same way as the usual ones, there is nevertheless a fundamental difference between these two kinds of translations. This follows from the fact that the generators  $\Pi_{cx}$  and  $\Pi_{cy}$  of the magnetic translations do not commute (the usual translations are based on the commuting generators  $p_x$  and  $p_y$ ). Because of this noncommutativity of  $\Pi_{cx}$  and  $\Pi_{cy}$ , it turns out to be impossible to choose the eigenfunctions (14) of the magnetic translations to be periodic in both  $\kappa_1$  and  $\kappa_2$ . The best one can do is to make  $\langle P | \vec{\kappa} \rangle$  periodic in one variable, say  $\kappa_1$ , but then they become Bloch periodic in  $\kappa_2$ . This is a general feature of the kq representation.<sup>16</sup> As a consequence of this, the eigenfunctions (19) are also Bloch periodic in  $\kappa_2$ . On the other hand, the Bloch function  $\psi_{m \vec{k}}$  can always be chosen to be periodic in both components of  $\vec{k}$ .<sup>35</sup> This difference between the magnetic Bloch functions (19) and the usual ones very strongly influence the definitions of localized functions for the corresponding problems, as is shown in Sec. IV.

#### **III. MAGNETIC ADAMS REPRESENTATION**

In the preceding section the magnetic Bloch functions for a rational magnetic field were derived. We now construct the representation based on these functions, which turns out to be analogous to the Adams representation in the Bloch theory.<sup>4</sup>

Let us write the orthogonality relations satisfied by the eigenfunctions (19). It can be easily shown that, for each  $\vec{\kappa}$ , the Hamiltonian in (20) is Hermitian, so that, using (15), one has

$$\int \int d\bar{P} dP \psi_{l\,\vec{\kappa}}^{*}(\bar{P},P)\psi_{l'\,\vec{\kappa}'}(\bar{P},P) = \delta_{l,l'}\hat{\Delta}(\vec{\kappa}-\vec{\kappa}') .$$
(22)
(22)

$$\sum_{l} \int d\vec{\kappa} \, \psi_{l\vec{\kappa}}^{*}(P,P) \psi_{l\vec{\kappa}}(P',P') = \delta(P-P') \,\delta(P-P') \,,$$
(23)

where the integral over  $\vec{\kappa}$  is performed in the region (17). Expressions for operators in the magnetic Adams representation are obtained by taking the matrix elements of the operator between the eigenfunctions (19). By using (14) and (22) we obtain then the representations of the operators in (6):

$$\langle l\vec{\kappa} | Q | l'\vec{\kappa}' \rangle = X_{ll'}(\vec{\kappa})\Delta(\vec{\kappa} - \vec{\kappa}') , \langle l\vec{\kappa} | \vec{P} | l'\vec{\kappa}' \rangle = Y_{ll'}(\vec{\kappa})\widehat{\Delta}(\vec{\kappa} - \vec{\kappa}') , \langle l\vec{\kappa} | Q | l'\vec{\kappa}' \rangle = i \frac{\partial}{\partial\kappa_2} \delta_{l,l'}\widehat{\Delta}(\vec{\kappa} - \vec{\kappa}') ,$$

$$\langle l\vec{\kappa} | P | l'\vec{\kappa}' \rangle = \left[ \frac{\beta}{i} \frac{\partial}{\partial\kappa_1} + \hbar\kappa_2 \right] \delta_{l,l'}\widehat{\Delta}(\vec{\kappa} - \vec{\kappa}') ,$$

$$(24)$$

where the following quantities have been introduced:

$$X_{ll'}(\vec{\kappa}) = \int d\vec{P} \, \varphi_{l\,\vec{\kappa}}^{*}(\vec{P}) i \hbar \frac{\partial}{\partial \vec{P}} \varphi_{l'\,\vec{\kappa}}(\vec{P}) ,$$
  

$$Y_{ll'}(\vec{\kappa}) = \int d\vec{P} \, \varphi_{l\,\vec{\kappa}}^{*}(\vec{P}) \vec{P} \varphi_{l'\,\vec{\kappa}}(\vec{P}) .$$
(25)

Because of the localization of  $\varphi_{l\vec{\kappa}}(\vec{P})$  in  $\vec{P}$ , mentioned in the preceding section, we may expect the quantities (25) to assume, in general, finite values. These can be calculated exactly in the potential-free case, where  $\varphi_{l\vec{\kappa}}(\vec{P}) = f_l(\vec{P})$ , an oscillator function. One has in this case

$$X_{ll'}^{(0)}(\vec{\kappa}) = i\sqrt{\hbar/2\beta}(\sqrt{l'}\delta_{l+1,l'} - \sqrt{l'+1}\delta_{l,l'+1}) ,$$
  
$$Y_{ll'}^{(0)}(\vec{\kappa}) = \frac{1}{2}\sqrt{\hbar\beta}(\sqrt{l'}\delta_{l+1,l'} + \sqrt{l'+1}\delta_{l,l'+1}) .$$

The matrices for  $x, y, p_x, p_y$  are obtained by inverting the transformation (6) and by using (24). One should compare the form of the matrix elements above with that of matrix elements in the ordinary Adams representation.<sup>4</sup> In particular, the fact that certain operators [such as Q and P in (24)] are diagonal in the magnetic band index is a consequence of the special structure of the eigenfunctions (19), which is quite different from that of usual Bloch functions.

Let  $\phi(\overline{P}, P)$  and  $B_l(\vec{\kappa})$  denote the same state in the  $\overline{PP}$  and the Adams representations, respectively. Using relations (22) and (23), together with (19) and (14), the following formulas connecting  $\phi(\overline{P}, P)$  with  $B_l(\vec{\kappa})$  are obtained:

$$B_{l}(\vec{\kappa}) = \sqrt{\hbar b_{1}/2\pi} \sum_{m} e^{i\kappa_{1}mb_{1}} \int d\bar{P} \,\varphi_{l\vec{\kappa}}^{*}(\bar{P}) \phi(\bar{P}, \hbar\kappa_{2} + \beta m b_{1}) , \qquad (26)$$

$$\phi(\overline{P},P) = \sum_{l} \int d\vec{\kappa} B_{l}(\vec{\kappa}) \psi_{l\vec{\kappa}}(\overline{P},P) = \sqrt{\hbar b_{1}/2\pi} \sum_{l} \int_{-\pi/b_{1}}^{\pi/b_{1}} d\kappa_{1} B_{l}(\kappa_{1},P/\hbar) \varphi_{l,\kappa_{1},P/\hbar}(\overline{P}) .$$

$$(27)$$

By using (26) we obtain the periodicity conditions obeyed by a wave function  $B_l(\vec{\kappa})$  in the Adams representation. They coincide with the conditions satisfied by a kq function<sup>16</sup>:

$$B_l(\kappa_1 + 2\pi/b_1, \kappa_2) = B_l(\vec{\kappa}) , \qquad (28a)$$

$$B_l(\kappa_1,\kappa_2+\beta b_1/\hbar) = e^{-\iota\kappa_1 b_1} B_l(\vec{\kappa}) . \qquad (28b)$$

We now consider the effect of magnetic translations on a wave function in the Adams representation. Defining a magnetic translation as in (4), one has

$$(-1)^{n_1 n_2} T(\vec{\mathbf{b}}_n) \equiv (-1)^{n_1 n_2} T(n_1 \vec{\mathbf{b}}_1 + n_2 \vec{\mathbf{b}}_2)$$
$$= T^{n_1} (\vec{\mathbf{b}}_1) T^{n_2} (\vec{\mathbf{b}}_2)$$
(29)

 $(n_1 \text{ and } n_2 \text{ are arbitrary integers})$ , which is derived by using the multiplication rule for magnetic translations<sup>3,11</sup> and relation (3). The operators (29) form a basic Abelian group<sup>11</sup> in the two-dimensional case. Since the magnetic Bloch functions (19), on which the Adams representation is based, are eigenfunctions of  $T(\vec{b}_1)$  and  $T(\vec{b}_2)$ , the elements of the group (29) are represented by the following matrices:

$$\langle l\vec{\kappa} | (-1)^{n_1 n_2} T(\vec{b}_n) | l'\vec{\kappa}' \rangle = e^{i\vec{\kappa}\cdot\vec{b}_n} \delta_{l,l'} \hat{\Delta}(\vec{\kappa}-\vec{\kappa}') .$$

This means that

$$(-1)^{n_1 n_2} T(\vec{\mathbf{b}}_n) B_l(\vec{\kappa}) = e^{i \vec{\kappa} \cdot \vec{\mathbf{b}}_n} B_l(\vec{\kappa}) .$$
(30)

We thus see that the effect of a magnetic translation (29) in the Adams representation is quite simple, and is expressed by multiplication by a  $\vec{\kappa}$ dependent phase factor. This is analogous to the effect of ordinary translations on a wave function in the Adams representation for the Bloch theory.<sup>4</sup>

#### **IV. LOCALIZATION IN A MAGNETIC FIELD**

The localization problem of a Bloch electron in a magnetic field has attracted attention ever since the very early stages of solid-state physics. In recent work<sup>36,37</sup> the problem of localization on von Neumann lattices was investigated in the framework of the kq representation. We show in this section how known results on von Neumann lattices can be applied for investigating the problem of localization in a magnetic field. Different sets of localized states will be considered, and a summary of their definitions is given for convenience in Table I.

We begin by reviewing earlier work on localized states in a magnetic field. A localized set of orbitals for the problem of a Bloch electron in a magnetic field was first introduced in the classical work of Peierls.<sup>22</sup> Peierls considered the limit of tight binding and attempted a solution in the form of a linear combination of atomic orbitals centered on lattice sites. In the absence of a magnetic field, and in the tight-binding limit, a satisfactory local solution of the Schrödinger equation is  $\phi(\vec{r} - \vec{t}_n)$ , namely, an atomic orbital centered on any lattice site  $\vec{t}_n$ . When  $\vec{H} \neq 0$ , one should apply to  $\phi(\vec{r})$  magnetic translations by lattice vectors in order to obtain local solutions. This gives the following orbitals:

$$T(-\vec{t}_{n})\phi(\vec{r}) = \exp[-(i/2\hbar)\vec{\beta} \times \vec{t}_{n} \cdot \vec{r}]$$
$$\times \phi(\vec{r} - \vec{t}_{n}), \qquad (31)$$

where  $T(-\vec{t}_n)$  is a magnetic translation by the lattice vector  $-\vec{t}_n$ . Thus one should multiply  $\phi(\vec{r}-\vec{t}_n)$  by the phase factors in (31) (known as the Peierls phase factors) in order to obtain local solutions in the case  $\vec{H} \neq 0$ . By using the orbitals (31)

TABLE I. Definitions of localized states.

Localized States	Definitions
Wannier functions	Eq. (46)
Peierls orbitals	Eq. (31)
Luttinger functions	Eq. (32)
Magnetic Wannier functions	Eqs. (33), (34), and (36) with (40)
Magnetic Wannier functions in the potential-free case	Eq. (42) or (44)
Dingle functions	Eq. (12)
Pippard network	Eqs. (35) and (37)

Peierls found that the energy eigenvalues within the tight-binding band  $E(\vec{k})$  could be obtained as eigenvalues of the operator  $E(\vec{\Pi}/\hbar)$  where  $\vec{\Pi}$  is the kinetic momentum (2).  $E(\vec{\Pi}/\hbar)$  is the effective Hamiltonian of the problem.

The results of Peierls were later derived by using Wannier functions instead of atomic orbitals,<sup>23,24,38</sup>

$$a_{m}(\vec{\mathbf{r}}; \mathbf{t}_{n}) = \exp[-(i/2\hbar)\vec{\beta} \times \mathbf{t}_{n} \cdot \vec{\mathbf{r}}] \times a_{m}(\vec{\mathbf{r}} - \vec{\mathbf{t}}_{n}), \qquad (32)$$

where  $a_m(\vec{r})$  is a Wannier function corresponding to a given Bloch band *m*. A common feature of the orbitals (31) and (32) is that they both form nonorthogonal sets of functions. However, while the atomic orbitals  $\phi(\vec{r} - \vec{t}_n)$  in (31) are nonorthogonal, the Wannier functions  $a_m(\vec{r} - \vec{t}_n)$  in (32) are known to form an orthogonal set. It is the presence of the Peierls phase factor in (32) that causes the nonorthogonality of the functions (32).

Wannier functions in the presence of a magnetic field can be obtained by using the localization ideas in the kq representation for perfect lattices.<sup>27</sup> These functions are calculated by treating the magnetic field as a perturbation to the Bloch problem, and their general form is

$$A_{mn}(\vec{r}) = a_m(\vec{r}; \vec{t}_n) + \sum_{s=1}^{\infty} H^s a_{mn}^{(s)}(\vec{r}) .$$
 (33)

At the lowest order in the perturbation expansion, the magnetic Wannier functions (33) reduce to the functions (32). Unlike (32), however, the functions (33) are orthogonal up to any desired order of  $\vec{H}$ .

Another definition of magnetic Wannier functions was given by Brown,<sup>25</sup> using the group-theoretical approach:

$$A(\vec{\mathbf{r}};\vec{\mathbf{t}}_n) = T(-\vec{\mathbf{t}}_n)A(\vec{\mathbf{r}}).$$
(34)

Here  $T(-\vec{t}_n)$  is a magnetic translation as in (31), and  $A(\vec{r})$  is a properly defined linear combination of eigenfunctions belonging to N magnetic bands [N is given by Eq. (3)]. According to Brown these N magnetic bands should result from the splitting of an isolated Bloch band in a magnetic field.

A common feature of all the magnetic orbitals (31)—(34) is that they are associated with the sites of the crystal lattice. In order to account for magnetic breakdown and related phenomena, Pippard<sup>9</sup> introduced a set of localized orbitals associated with the sites of magnetic lattice built on the  $b_n = n_1 b_1 + n_2 b_2$ . These orbitals are obtained by applying the magnetic translations (29) on a Dingle function (12) with p = 0 (corresponding to the classical circular trajectory in a magnetic field<sup>31</sup>). In the case of a rectangular lattice, the Pippard network of orbitals is then

$$(-1)^{n_1 n_2} T(\vec{b}_n) f_l(\vec{P}) f_0(P) = f_l(\vec{P}) e^{(i/\hbar)n_2 b_2 P} f_0(P - n_1 \beta b_1)$$
(35)

in the  $\overline{PP}$  representation, where we used (29) and (9). By a heuristic argument based on the degeneracy of Landau levels, Pippard showed that the set of functions (35) is sufficient to describe fully a given Landau level l and thus to account for its infinite degeneracy. The argument of Pippard was given a rigorous basis by Boon,<sup>20</sup> who showed that a Pippard network is completely analogous to a von Neumann lattice of coherent states.<sup>21</sup> The latter is the set of states obtained by operating on a harmonicoscillator ground state  $f_0(x)$  with translations on a lattice in the x-p phase plane, whose unit-cell area is h. It is well known that such a set of states is complete in  $L^{2}(x)$ .<sup>21</sup> This means that any squareintegrable function of x, which is orthogonal to all the states of the set, must essentially be the zero function. The close analogy of the von Neumann lattice with the Pippard network (35) is connected with the fact that the magnetic translations in (35) are simply translations on a lattice in the Q-P phase plane. The area of a unit cell of this lattice is h because of the basic relation (13), which expresses the fact that the magnetic cell  $\vec{b}_1 - \vec{b}_2$  encloses exactly one quantum of flux, hc/e. It follows that the set of states in (35) [without the factor  $f_l(\overline{P})$ ] is complete in  $L^{2}(P)$ . From the discussion following formula (10), we may interpret this by saying that the Pippard network (35) spans the Landau level *l*. This gives a precise meaning to the statement of Pippard. It should be pointed out that one may also construct complete Pippard networks from "excited" Dingle functions [namely, those with p > 0 in (12)].<sup>20</sup> This is completely analogous to von Neumann lattices built on excited harmonic-oscillator states.<sup>37</sup>

Let us now show that in the presence of a periodic potential leading to a broadening of the Landau levels, it is also possible to define a Pippard network of magnetic orbitals spanning a given magnetic band. Consider the most general linear combination of eigenfunctions belonging to magnetic band l'. From the first equality in (27) this is

$$A_{l'}(\overline{P},P) = \int d\vec{\kappa} B_{l'}(\vec{\kappa}) \psi_{l'\vec{\kappa}}(\overline{P},P) , \qquad (36)$$

where  $B_{l'}(\vec{\kappa})$  is a general function satisfying the periodicity conditions (28). In the Adams representation the orbital (36) reads simply  $\delta_{l,l'}B_{l'}(\vec{\kappa})$ . By operating with the magnetic translations (29) and using (30), we obtain the set of functions

$$(-1)^{n_1 n_2} T(\vec{\mathbf{b}}_n) \delta_{l,l'} B_{l'}(\vec{\kappa}) = \delta_{l,l'} e^{i \vec{\kappa} \cdot \vec{\mathbf{b}}_n} B_{l'}(\vec{\kappa}) .$$
(37)

We now show that the set (37) is complete, relative to magnetic band l'. Let  $G(\vec{\kappa})$  be a function (in the Adams representation) that belongs to the magnetic band l', which is orthogonal to all the functions (37). We then have

$$\int d\vec{\kappa} G^*(\vec{\kappa}) e^{i\vec{\kappa}\cdot\vec{b}_n} B_{l'}(\vec{\kappa}) = 0$$
(38)

for all  $\vec{b}_n$ . Now, since the integral in (38) gives the Fourier coefficients of the periodic function  $G^*(\vec{\kappa})B_{l'}(\vec{\kappa})$ , this latter product must vanish, and we then obtain  $G(\vec{\kappa})=0$ .<sup>39</sup> This means that the set (37) is complete, relative to magnetic band l'.

A complete description of a single magnetic band is thus provided by the Pippard network of orbitals (37), which are associated with the sites  $\vec{b}_n$  of the magnetic lattice. Orbitals associated with general sites of the crystal lattice become superfluous in this description.

The orbitals (37) may be interpreted as magnetic

Wannier functions for the problem if, in addition to their completeness, they also form an orthogonal set of functions. From the requirement of orthogonality of (37), it follows that (for  $n \neq n'$ )

$$\int d\vec{\kappa} e^{i\vec{\kappa}\cdot(\vec{b}_n-\vec{b}_{n'})} |B_{l'}(\vec{\kappa})|^2 = 0.$$
(39)

Relation (39) means that  $|B_{l'}(\vec{\kappa})|$  has to be a constant and therefore

$$B_{l'}(\vec{\kappa}) = C e^{i\tau(\vec{\kappa})} , \qquad (40)$$

where C is some constant and  $\tau(\vec{\kappa})$  is a real function of  $\vec{\kappa}$ . The constant C will be chosen as  $\sqrt{\hbar/2\pi\beta}$  in order to normalize (40) in the usual sense [the integral in (39) is equal to 1 for n = n']. The orbitals (37), with  $B_{l'}(\vec{\kappa})$  given by (40), form a complete set of magnetic Wannier functions spanning the magnetic band l'. This is in full analogy with a general von Neumann lattice of states in the kq representation.<sup>36,37</sup>

It can be easily shown that any continuous function of  $\vec{\kappa}$  that satisfies the periodicity conditions (28) must vanish somewhere. The proof of this statement is analogous to that given for a general wave function in the kq representation.<sup>37</sup> Since the function  $B_{l'}(\vec{\kappa})$  in (40), corresponding to the magnetic Wannier functions, cannot vanish because of its exponential nature, we conclude that it must be discontinuous. For example, one may choose in (40) (with  $C = \sqrt{\hbar/2\pi\beta}$ ) the following expression<sup>36,40</sup>:

$$B_{l'}(\vec{\kappa}) = \sqrt{\hbar/2\pi\beta} \exp[-i(\hbar/\beta)\overline{\kappa}_1\kappa_2] , \qquad (41)$$

where  $\overline{\kappa}_1 = \kappa_1$ , for  $-\pi/b_1 \le \kappa_1 < \pi/b_1$ , and is periodically continued beyond this interval (a sawlike function). It is easily checked that (41) satisfies the conditions (28), but it is, of course, discontinuous in  $\vec{\kappa}$ . The orbital (36) with the choice (41) for  $B_{l'}(\vec{\kappa})$  is easily calculated in the potential-free case [the eigenfunctions  $\psi_{l'\vec{\kappa}}(\overline{P}, P)$  being given by (16)]. We obtain

$$A_{I'}(\bar{P}, P) = (\bar{P})\sqrt{b_2/h} f_{I'} \frac{\sin(\pi P/\beta b_1)}{(\pi P/\beta b_1)} .$$
 (42)

It is of interest to have the orbital (42) written in the xy representation. By using the transformation (A4) between the  $\overline{PP}$  and the xy representations, we get

$$A_{l'}(x,y) = \frac{1}{2} \sqrt{\beta/b_1} e^{-i(\beta/2\hbar)xy} \int_{-1}^{1} dz \exp[i(\pi/b_1)zx] f_{l'}((\pi\hbar/b_1)z - \beta y) .$$
(43)

In order to better display the localization of the function (43), it is convenient to express it in a different form. Being an oscillator eigenfunction of the Hamiltonian  $H_0$  in (8),  $f_{I'}(\bar{P})$  depends on  $\bar{P}$  through the dimensionless variable  $u = \bar{P}/\sqrt{\hbar\beta}$ . Writing thus  $f_{I'}(\bar{P}) = g_{I'}(u)$ , and expanding  $g_{I'}(u)$  in a Taylor series around the point  $u_0 = -\sqrt{\beta/\hbar}y$ , we obtain the following expression:

$$A_{l'}(x,y) = \sqrt{2\beta/\pi b_2} e^{-i(\beta/2\hbar)xy} \sum_{n=0}^{\infty} \frac{(-ib)^n}{n!} \frac{\partial^n}{\partial x^n} \left[ \frac{\sin(\pi x/b_1)}{(x/b)} \right] \frac{\partial^n g_{l'}(u)}{\partial u^n} \bigg|_{u=-y/b},$$
(44)

where  $b = \sqrt{\hbar/\beta}$  is equal in magnitude to the classical cyclotron radius for the ground-state energy  $\hbar\omega_c/2$ . The sum in (44) converges for all x and y and is an expansion in powers of the variable b/x, which is small for  $x \gg b$ . It can be easily seen then that  $A_{l'}(x,y)$  is well localized in the y direction (like a harmonic-oscillator function), and falls off essentially as 1/x when  $|x| \to \infty$ .

This localization of the magnetic Wannier function (44) should be compared with that of the Dingle functions (35). The latter correspond to the classical magnetic orbits, and have a harmonic-oscillator localization in all directions of the x-y plane.<sup>31</sup> The classical features of the Dingle functions (35) are expressed by the fact that they assume the smallest undeterminancy possible in the location of the orbit center  $\Delta x_0 \Delta y_0 = \hbar/2\beta^{20,31}$  For the magnetic Wannier function (44) [or (42)], on the other hand, one can show that  $\Delta x_0 \Delta y_0 = \infty$ , and so it is very far from classical states.

The value of  $\Delta x_0 \Delta y_0$  for the orbital (36) does not depend on the detailed magnetic band structure (or the periodic potential), but only on the expansion coefficient  $B_{l'}(\vec{\kappa})$ . This is because the matrices for  $Q = y_0$  and  $P = -\beta x_0$  in the Adams representation [see (24)] do not depend on expressions involving the dynamical part  $\varphi_{I\vec{r}}(\vec{P})$  of the eigenfunctions (19). These matrices are also completely analogous to the expressions for x and p in the kg representation.<sup>16</sup> Recently,<sup>37</sup> this representation was used to show that orthogonal states on a von Neumann lattice are necessarily noncoherent, namely  $\Delta x \ \Delta p = \infty$  for these states. By means of the Adams representation one may prove similarly that Pippard networks of magnetic Wannier functions are characterized by an infinite value of  $\Delta x_0 \Delta y_0$ , even in the presence of a periodic potential. In other words, orbitals on a Pippard network with  $\Delta x_0 \Delta y_0 < \infty$  are necessarily nonorthogonal. An extreme example is the Pippard network of Dingle functions (35), which assume the smallest value of  $\Delta x_0 \Delta y_0$  but are known to form a nonorthogonal set of functions.9,20

This difference between Pippard networks built on Dingle functions and on magnetic Wannier functions is connected with the analytic properties of the function  $B_{l'}(\vec{\kappa})$  in the two cases. Consider the function  $B_{l'}(\vec{\kappa})$  in (37) corresponding to a Pippard network of Dingle functions. Substituting (12), with p = 0, into Eq. (26) [with  $\varphi_{l\vec{\kappa}}(\vec{P}) = f_{l'}(\vec{P})$ ], we find

$$B_{I'}(\vec{\kappa}) = \left[\frac{b_1^3 b_2}{8\pi^4}\right]^{1/4} \exp\left[\frac{-\hbar}{2\beta}\kappa_2^2\right] \vartheta_3(z \mid \tau) , \quad (45)$$

where  $z = b_1(\kappa_1 + i\kappa_2)/2$ ,  $\tau = ib_1/b_2$ , and  $\vartheta_3(z \mid \tau)$  is a theta function.<sup>41</sup> While  $B_{l'}(\vec{\kappa})$  in (45) is an entire function of  $\vec{\kappa}$ , the function  $B_{l'}(\vec{\kappa})$  in (40) and (41) (corresponding to the magnetic Wannier functions) is not even continuous.

It is interesting to note that the orbital (36) with  $B_{l'}(\vec{\kappa})$  given by (45) assumes the minimal undeterminancy  $\Delta x_0 \Delta y_0$  even in the presence of a periodic potential. The problem of defining a wave function with a good localization in the orbit center for a Bloch electron in a magnetic field was first considered by Chambers.<sup>24</sup> He constructed such a wave function in the framework of an effective-Hamiltonian approach and showed its localization by means of the WKB and other approximations. Here we have an exact result. The set of orbitals (37), with  $B_{l'}(\vec{\kappa})$  given by (45), assumes the smallest value of  $\Delta x_0 \Delta y_0$  and forms a nonorthogonal set of functions spanning the magnetic band l'. This set is then completely analogous to the Pippard network of Dingle functions (35) in the potential-free case.

It is instructive to compare the concepts of localization and orthogonality of magnetic orbitals with the corresponding concepts in the Bloch theory  $(\vec{H}=0)$ . In the latter theory one has the notion of a Wannier function,<sup>28</sup> defined as

$$a_m(\vec{\mathbf{r}}) = \frac{1}{\sqrt{V_b}} \int d\vec{\mathbf{k}} \,\psi_{m\,\vec{\mathbf{k}}}(\vec{\mathbf{r}}) \,, \tag{46}$$

where  $V_b$  is the volume of a unit cell of the reciprocal lattice,  $\psi_{m\,\vec{k}}(\vec{r})$  is a Bloch function corresponding to band *m*, and the integration is over  $V_b$ . By operating with ordinary translations on the crystal lattice, one generates from (46) an orthogonal set of functions  $a_m(\vec{r}-\vec{t}_n)$ , which span the band *m* in the following sense:

$$\psi_{m\,\vec{\mathbf{k}}}(\vec{\mathbf{r}}) = \frac{1}{\sqrt{V_b}} \sum_n e^{i\,\vec{\mathbf{k}}\cdot\vec{\mathbf{t}}_n} a_m(\vec{\mathbf{r}}-\vec{\mathbf{t}}_n) \; .$$

It is well known that the Wannier function (46) can always be chosen to be localized in space, in the sense of an exponential decay.<sup>29,30</sup> Thus, in the onedimensional case, for example, the Wannier function falls off exponentially as  $\exp(-\bar{h}_m |x|)$ , where  $\bar{h}_m$ , known as the degree of localization, is the halfwidth of the strip of analyticity of the Bloch functions  $\psi_{mk}(x)$  in the complex k plane.<sup>29</sup> This localization of the Wannier functions should be compared with that of the magnetic Wannier functions generated from the orbital (42) [or (44)]. The latter is rather poorly localized in one direction of space (with a falloff as 1/P or as 1/x).

The basic reason for the difference in localization between the Wannier functions in the cases  $\vec{H}=0$ and  $\vec{H}\neq 0$  is as follows. Wannier functions are generated from a single function by operating on it with ordinary translations, while magnetic orbitals are generated by magnetic translations, which are actually translations in a phase space. As we have already seen in Sec. II, from this difference between the two kinds of translations it follows that Bloch functions can be made strictly periodic in k space,<sup>35</sup> while the eigenfunctions (19) must satisfy the periodicity conditions (21). It is just because of these latter conditions that  $B_{l'}(\vec{\kappa})$  in (40) (which corresponds to the magnetic Wannier functions) must be a discontinuous function of  $\vec{\kappa}$ , and this then leads to poorly localized orbitals. The difference between ordinary and magnetic translations is well demonstrated by the Luttinger functions (32). These differ from the  $a_m(\vec{r} - \vec{t}_n)$  by the Peierls phase factors, and as such, they assume the same degree of localization of the Wannier functions. Unlike Wannier functions, however, the functions (32) do not form an orthogonal set<sup>23</sup> just because of the presence of the Peierls phase factors, which make all the difference between ordinary and magnetic translations.

## **V. CONCLUSIONS**

Magnetic translations are associated with the degree of freedom for the orbit center and are essentially translations in a phase space. Because of this fact, Bloch functions in a magnetic field behave like kq functions in one coordinate of the orbit center. Correspondingly, the Adams representation based on these functions reduces to a kq representation when restricted to a single magnetic band.

In this paper the magnetic Adams representation was developed and used for investigating the problem of localization of a Bloch electron in a magnetic field. A Pippard network of orbitals was introduced, spanning a single magnetic band. As in the case of a general von Neumann lattice of states<sup>36,37</sup> this network is generated by a discrete set of translations in a phase space (the magnetic translations). The analogy of the magnetic Adams representation with the kq representation is used in order to apply known results on von Neumann lattices<sup>36,37</sup> to Pippard networks of magnetic orbitals. In particular, it is shown that exponential localization of magnetic orbitals is excluded by their orthogonality.

It does not seem possible, therefore, to choose magnetic Wannier functions that are both orthogonal and atomiclike (or similar to ordinary Wannier functions). For example, the generalized Wannier functions (34), which are chosen to be orthogonal, cannot be assumed, contrary to what is claimed in Ref. 25, to be also atomiclike. The arguments in Ref. 25 make use of a conjecture that an isolated Bloch band splits into N magnetic bands when a magnetic field is turned on [N is given by Eq. (3)].

This conjecture, which has never been proved, was based on the fact that the magnetic Brillouin zone is N times smaller than the Brillouin zone of the same crystal for a zero magnetic field. Correspondingly, the magnetic band has N times fewer states than a Bloch band. However, the magnetic operator symmetry is not a subgroup of the Bloch symmetry,<sup>11</sup> and one has therefore no grounds to claim that a Bloch band should split into N magnetic subbands when  $\vec{H}\neq 0$ . As a matter of fact the splitting into Nsubbands was confirmed only approximately for a tight-binding model and for low magnetic fields (large N).<sup>42</sup> In the nearly-free-electron case (when band overlapping takes place) the splitting may deviate considerably from N.<sup>26,43</sup>

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#### APPENDIX

The problem of an electron in a uniform magnetic field provides a good example<sup>19</sup> for the use of canonical transformation methods in quantum mechanics.<sup>44</sup> In Sec. II of this paper these methods were used in order to introduce a convenient representation for describing the problem of a Bloch electron in a magnetic field, the  $\overline{PP}$  representation. The unitary transformation between wave functions written in the  $\overline{PP}$  and in the xy representations can be found by means of formula (3.27) of Ref. 44. In order to use that formula, let us recall first the general form of a canonical transformation [Eq. (3.2) of Ref. 44],

$$\overline{x}_i = a_{ij} x_j + b_{ij} p_j ,$$

$$\overline{p}_i = c_{ij} x_j + d_{ij} p_j ,$$
(A1)

where i, j = 1, ..., N, and the  $N \times N$  matrices  $\underline{A} = ||a_{ij}||, \underline{B} = ||b_{ij}||$ , etc., are submatrices of

$$\underline{S} = \begin{bmatrix} \underline{A} & \underline{B} \\ \underline{C} & \underline{D} \end{bmatrix}$$
(A2)

where  $\underline{S}$  is an element of the 2N-dimensional real sympletic group Sp(2N). The unitary transformation between the  $\overline{x}_i$  and the  $x_i$  representations is given by formula (3.27) of Ref. 44, and is

$$\langle X' | U | X'' \rangle = \left[ (2\pi\hbar)^N | \det \underline{B} | \right]^{-1/2} \exp\left[ \frac{-i}{2\hbar} (\widetilde{X}' \underline{B}^{-1} \underline{A} X' - 2\widetilde{X}' \underline{B}^{-1} X'' + \widetilde{X}'' \underline{D} \underline{B}^{-1} X'') \right],$$
(A3)

where  $\widetilde{X}'$  denotes the N-dimensional row vector  $(x_1, \ldots, x_N)$  and the tilde over a vector stands for transposition. The vector  $\widetilde{X}''$  in (A3) corresponds to the transformed-coordinate row vector  $(\overline{x}_1, \ldots, \overline{x}_N)$ . In our case the canonical transformation is given by (6). We have N=2, and make the identifications  $\widetilde{X}''=(\overline{x}_1,\overline{x}_2)=(-\overline{P},-P)$ ,  $\widetilde{X}'=(x_1,x_2)=(x,y)$ . Because of (7) the operators  $(\overline{x}_1,\overline{x}_2)=(-\overline{P},-P)$  behave as position operators, and formula (A3) can then be used to connect between the  $\overline{PP}$  and the xy representations. By making the further identifications  $(\overline{p}_1,\overline{p}_2)=(\overline{Q},Q)$ ,  $(p_1,p_2)=(p_x,p_y)$ , and comparing (6) with (A1), the desired transformation is obtained:

$$\Psi(x,y) = \frac{1}{2\pi\hbar} \int \int d\bar{P} \, dP \exp\left[\frac{i\beta}{\hbar} \left[\frac{xy}{2} + \frac{\bar{P}P}{\beta^2} + \frac{\bar{P}x}{\beta} + \frac{Py}{\beta}\right]\right] \phi(\bar{P},P) , \qquad (A4)$$

where  $\Psi(x,y)$  and  $\phi(\overline{P},P)$  represent the state in the xy and the  $\overline{PP}$  representations, respectively.

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